Irreducible bases in icosahedral group space

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The irreducible bases in the icosahedral group space are calculated explicitly by reducing the regular representation. The symmetry adapted bases of the system with **I** or $\mathbf{I}_h$ symmetry can be calculated easily and generally by applying those irreducible bases to wavefunctions of the system, if they are not vanishing. As examples, the submatrices of the Hückel Hamiltonians for Carbon-60 and Carbon-240 are re-calculated by the irreducible bases.

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I. INTRODUCTION

Fullerences (Kroto 1988, Huffman 1991, Pennis 1991), such as $B_{12}H_{12}$, $C_{20}H_{20}$ and C_{60}, are intriguing cage-like molecules of carbon atoms with the icosahedral symmetry. This discovery (Rohlfing *et al.* 1984, Kroto *et al.* 1985, Weeks and Harter 1989) has greatly drawn attentions of chemists and physicists (Deng and Yang 1992, Chou and Yang 1993, Friedberg and Lee 1992). With the development of experimental techniques in high resolution spectroscopy, many new data on vibrational spectra of polyatomic molecules with the symmetry $\mathbf{I}_h$ were observed and analyzed (Negri and Orlandi 1996, Olthof *et al.* 1996, Giannozzi and Baroni 1994, Schettino *et al.* 1994, Gunnarsson *et al.* 1995, Doye and Wales 1996, Wang *et al.* 1996, Tang *et al.* 1996, Tang and Huang 1997). The vibrational modes, the force fields, and the spin-orbit coupling coefficients for icosahedral molecules were studied in some detail (Clougherty and Gorman 1996, Martínez-Torres *et al.* 1996, Varga *et al.* 1996, Fowler and Ceulemans 1985).

As is well known, symmetry analysis provides a powerful tool for classifying energy levels and organizing experimental data. In explaining the vibrational spectra of polyatomic molecules, the symmetry adapted bases (SAB) play an important role in simplifying the calculations (Lemus and Frank 1994, Ma *et al.* 1996, Chen *et al.* 1996). The SAB are defined as the orthogonal bases that belong to given rows of given irreducible representations of the symmetry group. In those studies, SAB of the system with the $\mathbf{I}_h$ symmetry were widely used. Therefore, the properties of the $\mathbf{I}_h$ group are worthy to be studied in some detail, although the dimension of the $\mathbf{I}_h$ group space is 120.

Early works on $\mathbf{I}$ group are mainly concerned with the construction of the representations of $\mathbf{I}$ subduced by D^ℓ of SO(3) group and the 3j- and 6j-symbols (McLellan 1961, Golding 1973, Pooler 1980, Brown 1987). Liu-Ping-Chen (1990) enumerated the 60 elements of icosahedral group $\mathbf{I}$, listed its group table, and calculated the irreducible representation matrices of all the 60 elements explicitly. The character tables of the point groups and the double point groups were listed (Altmann and Herzig 1994, Balasubramanian 1996). Recently, Chen and Ping (1997) constructed the point-group symmetrized boson representation, and gave the explicit expressions of the SAB for seven important cases of the molecule $B_{12}H_{12}$.

As another approach, in this paper we will explicitly calculate the irreducible bases $\psi^\Gamma_{\mu\nu}$ in the group spaces of $\mathbf{I}$ and $\mathbf{I}_h$ by reducing the regular representation of $\mathbf{I}$:

$$R\psi^\Gamma_{\mu\nu} = \sum_\rho \psi^\Gamma_{\rho\nu} D^\Gamma_{\rho\mu}(R), \qquad \psi^\Gamma_{\mu\nu} R = \sum_\rho D^\Gamma_{\nu\rho}(R) \psi^\Gamma_{\mu\rho}, \qquad R \in \mathbf{I}. \tag{1}$$

where D^Γ is an irreducible representation of $\mathbf{I}$, and $\psi^\Gamma_{\mu\nu}$ is a combination of the group elements. Applying those irreducible bases to any function $F(x)$, if it is not vanishing, one will obtain the SAB $\psi^\Gamma_{\mu\nu} F(x)$:

$$R\left\{\psi^\Gamma_{\mu\nu} F(x)\right\} = \sum_\rho \left\{\psi^\Gamma_{\rho\nu} F(x)\right\} D^\Gamma_{\rho\mu}(R). \tag{2}$$

It is an unified and straightforward way to calculate the SAB of the system with the $\mathbf{I}_h$ symmetry.

By the way, we would like to point out that the rank of group **I** is two, not three (McLellan 1961, Liu *et al.* 1990, Lomont 1959). It means that all 60 elements of **I** can be expressed as the products of only two generators.

The plan of this paper is as follows. In Sec. II we will give our notations. In Sec. III the irreducible bases in the **I** group space are calculated explicitly, and the irreducible bases of $\mathbf{I}_h$ are easy to be calculated from those of **I**. Three examples are given to explain how to calculate the SAB in terms of those irreducible bases. A short conclusion is given in Sec. IV.

II. NOTATIONS AND GENERATORS OF GROUP I

A regular icosahedron is shown in Fig.1. The vertices on the upper part are labeled by A_j, $0 \le j \le 5$, and their opposite vertices by B_j. The z and y axes point from the center O to A_0 and the midpoint of A_2B_5, respectively.

Fig. 1.

The group **I** has 6 five-fold axes, 10 three-fold axes, and 15 two-fold axes. One of the five-fold axes directs along z axis, and the rest point from B_j to A_j ($1 \le j \le 5$) with the polar angle θ_1 and azimuthal angles $\varphi_j^{(1)}$. The rotations through $2\pi/5$ around those five-fold axes are denoted by T_j, $0 \le j \le 5$. The three-fold axes join the centers of two opposite faces. The polar angles of the first and last 5 axes are denoted by θ_2 and θ_3, respectively, and the azimuthal angles by $\varphi_j^{(2)}$. The rotations through $2\pi/3$ around those three-fold axes are denoted by R_j, $1 \le j \le 10$. The two-fold axes join the midpoints of two opposite edges. The polar and azimuthal angles of the first, next and last 5 axes are θ_4, $\varphi_j^{(1)}$, θ_5, $\varphi_j^{(2)}$, π, and $\varphi_j^{(3)}$, respectively. The rotations through π around those two-fold axes are denoted by S_j, $1 \le j \le 15$. Those angles θ_i and $\varphi_j^{(i)}$ are given as follows:

$$\begin{array}{lll}
\tan\theta_1 = 2, & \tan\theta_2 = 3-\sqrt{5} = 2p^2, & \tan\theta_3 = 3+\sqrt{5} = 2p^{-2}, \\
\tan\theta_4 = \left(\sqrt{5}-1\right)/2 = p, & \tan\theta_5 = \left(\sqrt{5}+1\right)/2 = p^{-1}, & \\
\varphi_j^{(1)} = 2(j-1)\pi/5, & \varphi_j^{(2)} = (2j-1)\pi/5, & \varphi_j^{(3)} = (4j-3)\pi/10, \\
p = \eta+\eta^{-1}, & p^{-1} = 1+\eta+\eta^{-1}, & \eta = \exp(-i2\pi/5).
\end{array} \tag{3}$$

It is easy to see from Fig. 1 that 12 elements E, S_8, S_{12}, S_1, $R_6^{\pm1}$, $R_2^{\mp1}$, $R_4^{\pm1}$ and $R_{10}^{\mp1}$ construct a subgroup T. Now, any element R of **I** can be expressed as a product of T_0^a and an element $R_6^b S_1^c S_{12}^d$ of the subgroup T:

$$R = T_0^a R_6^b S_1^c S_{12}^d, \tag{4}$$

Owing to the relations:

$$R_6 = S_1 T_0^2 S_1 T_0^4, \quad S_{12} = R_6^2 S_1 R_6, \tag{5}$$

T_0 and S_1 are the generators of group **I**. The rank of **I** is two.

III. IRREDUCIBLE BASES IN I AND $\mathbf{I}_h$ GROUP SPACES

It is convenient to choose the irreducible representations of $\mathbf{I}$ such that the representation matrices of one generator T_0 are diagonal. Assume that the bases $\Phi_{\mu\nu}$ in the $\mathbf{I}$ group space are the eigenstates of left-action and right-action of T_0:

$$\begin{aligned} &T_0\ \Phi_{\mu\nu} = \eta^{\mu}\Phi_{\mu\nu}, \qquad &&\Phi_{\mu\nu}\ T_0 = \eta^{\nu}\Phi_{\mu\nu}, \\ &\eta = \exp(-i2\pi/5), \qquad &&\mu,\ \ \nu\ \ \mathrm{mod}\ \ 5\ . \end{aligned} \tag{6}$$

The eigenstates can be easily calculated by the projection operator P_μ (see p.113 in Hamermesh 1962):

$$\Phi_{\mu\nu} = c\ P_\mu\ R\ P_\nu, \qquad P_\mu = \frac{1}{5}\sum_{\lambda=-2}^{2}\ \eta^{-\mu\lambda}\ T_0^{\lambda}, \tag{7}$$

where c is a normalization factor. The choice of the group element R in (7) will not affect the results except for the factor c. In the following we choose E, S_{11}, S_5 and S_{10} as the group element R, respectively, and obtain four independent sets of bases $\Phi^{(i)}_{\mu\nu}$:

$$\begin{aligned} \Phi^{(1)}_{\mu\mu} &= \left(E + \eta^{-\mu}T_0 + \eta^{-2\mu}T_0^2 + \eta^{2\mu}T_0^3 + \eta^{\mu}T_0^4\right)/\sqrt{5}\ , \\ \Phi^{(2)}_{\mu\overline{\mu}} &= \left(S_{11} + \eta^{-\mu}S_{14} + \eta^{-2\mu}S_{12} + \eta^{2\mu}S_{15} + \eta^{\mu}S_{13}\right)/\sqrt{5}\ , \\ \Phi^{(3)}_{\mu\nu} &= \left\{\left(S_5 + \eta^{-\mu}R_5^2 + \eta^{-2\mu}T_1^4 + \eta^{2\mu}T_4 + \eta^{\mu}R_4\right)\right. \\ &\quad + \ \eta^{(\mu-\nu)}\left(S_4 + \eta^{-\mu}R_4^2 + \eta^{-2\mu}T_5^4 + \eta^{2\mu}T_3 + \eta^{\mu}R_3\right) \\ &\quad + \ \eta^{2(\mu-\nu)}\left(S_3 + \eta^{-\mu}R_3^2 + \eta^{-2\mu}T_4^4 + \eta^{2\mu}T_2 + \eta^{\mu}R_2\right) \\ &\quad + \ \eta^{-2(\mu-\nu)}\left(S_2 + \eta^{-\mu}R_2^2 + \eta^{-2\mu}T_3^4 + \eta^{2\mu}T_1 + \eta^{\mu}R_1\right) \\ &\quad + \ \left.\eta^{-(\mu-\nu)}\left(S_1 + \eta^{-\mu}R_1^2 + \eta^{-2\mu}T_2^4 + \eta^{2\mu}T_5 + \eta^{\mu}R_5\right)\right\}/5\ , \\ \Phi^{(4)}_{\mu\nu} &= \left\{\left(S_{10} + \eta^{-\mu}T_1^3 + \eta^{-2\mu}R_6^2 + \eta^{2\mu}R_9 + \eta^{\mu}T_5^2\right)\right. \\ &\quad + \ \eta^{(\mu-\nu)}\left(S_9 + \eta^{-\mu}T_5^3 + \eta^{-2\mu}R_{10}^2 + \eta^{2\mu}R_8 + \eta^{\mu}T_4^2\right) \\ &\quad + \ \eta^{2(\mu-\nu)}\left(S_8 + \eta^{-\mu}T_4^3 + \eta^{-2\mu}R_9^2 + \eta^{2\mu}R_7 + \eta^{\mu}T_3^2\right) \\ &\quad + \ \eta^{-2(\mu-\nu)}\left(S_7 + \eta^{-\mu}T_3^3 + \eta^{-2\mu}R_8^2 + \eta^{2\mu}R_6 + \eta^{\mu}T_2^2\right) \\ &\quad + \ \left.\eta^{-(\mu-\nu)}\left(S_6 + \eta^{-\mu}T_2^3 + \eta^{-2\mu}R_7^2 + \eta^{2\mu}R_{10} + \eta^{\mu}T_1^2\right)\right\}/5\ , \end{aligned} \tag{8}$$

where and hereafter the subscript $\overline{\mu}$ denotes $-\mu$. Those bases $\Phi^{(i)}_{\mu\nu}$ should be combined into the irreducible bases $\psi^{\Gamma}_{\mu\nu}$ that belong to the given irreducible representation Γ. The combinations can be determined from the condition that $\psi^{\Gamma}_{\mu\nu}$ should be the eigenstate of a class operator W, which was called CSCO-I by Chen and Ping (1997). The eigenvalues α_Γ can be calculated from the characters in the irreducible representations Γ (see (3-170) in Hamermesh 1962):

$$\begin{aligned} &W = \sum_{j=0}^{5}\ \left(T_j + T_j^4\right), \qquad &&W\ \psi^{\Gamma}_{\mu\nu} = \psi^{\Gamma}_{\mu\nu}\ W = \alpha_\Gamma\ \psi^{\Gamma}_{\mu\nu}, \\ &\alpha_A = 12, \quad \alpha_{T_1} = 4p^{-1}, \quad \alpha_{T_2} = -4p, \quad \alpha_G = -3, \quad \alpha_H = 0. \end{aligned} \tag{9}$$

Now we calculate the matrix form of W in the bases $\Phi^{(i)}_{\mu\nu}$, and diagonalize it. $\psi^{\Gamma}_{\mu\nu}$ are just the eigenvectors of the matrix form of W:

$$\psi^{\Gamma}_{\mu\nu} = N^{-1/2}\ \sum_{i=1}^{4}\ C_i\ \Phi^{(i)}_{\mu\nu}, \tag{10}$$

where N is the normalization factor. In those bases $\psi^{\Gamma}_{\mu\nu}$, the representation matrices are diagonal with the diagonal elements η^{μ} (see (6)). In principle, each $\psi^{\Gamma}_{\mu\nu}$ contains a free phase, and the representation matrices of another generator S_1 depend upon the choice of phases. We choose the phases such that the representation matrices of S_1 are as follows:

$$D^{A}(S_1) = 1, \qquad D^{T_1}(S_1) = \frac{1}{\sqrt{5}} \begin{pmatrix} -p^{-1} & -\sqrt{2} & -p \\ -\sqrt{2} & 1 & \sqrt{2} \\ -p & \sqrt{2} & -p^{-1} \end{pmatrix},$$

$$D^{T_2}(S_1) = \frac{1}{\sqrt{5}} \begin{pmatrix} -p & \sqrt{2} & p^{-1} \\ \sqrt{2} & -1 & \sqrt{2} \\ p^{-1} & \sqrt{2} & -p \end{pmatrix}, \quad D^{G}(S_1) = \frac{1}{\sqrt{5}} \begin{pmatrix} -1 & -p & -p^{-1} & 1 \\ -p & 1 & -1 & -p^{-1} \\ -p^{-1} & -1 & 1 & -p \\ 1 & -p^{-1} & -p & -1 \end{pmatrix},$$

$$D^{H}(S_1) = \frac{1}{5} \begin{pmatrix} p^{-2} & 2p^{-1} & \sqrt{6} & 2p & p^{2} \\ 2p^{-1} & p^{2} & -\sqrt{6} & -p^{-2} & -2p \\ \sqrt{6} & -\sqrt{6} & -1 & \sqrt{6} & \sqrt{6} \\ 2p & -p^{-2} & \sqrt{6} & p^{2} & -2p^{-1} \\ p^{2} & -2p & \sqrt{6} & -2p^{-1} & p^{-2} \end{pmatrix}. \tag{11}$$

where the row (column) indices μ of the irreducible representations Γ are put in the following order: 0 for A, 1, 0, and $\overline{1}$ for T_1, 2, 0, and $\overline{2}$ for T_2, 2, 1, $\overline{1}$, and $\overline{2}$ for G, and 2, 1, 0, $\overline{1}$, and $\overline{2}$ for H. The representation matrices of some irreducible representations of $\mathbf{I}$ coincide with those in the subduced representations of D^{ℓ} of SO(3):

$$D^{0}(R) = D^{A}(R), \quad D^{1}(R) = D^{T_1}(R), \quad D^{2}(R) = D^{H}(R),$$
$$X^{-1} D^{3}(R) X = D^{T_2}(R) \oplus D^{G}(R), \quad R \in \mathbf{I},$$
$$X = \begin{pmatrix} 0 & 0 & -\sqrt{2/5} & 0 & 0 & 0 & \sqrt{3/5} \\ \sqrt{3/5} & 0 & 0 & -\sqrt{2/5} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & \sqrt{3/5} & 0 & 0 & 0 & \sqrt{2/5} \\ \sqrt{2/5} & 0 & 0 & \sqrt{3/5} & 0 & 0 & 0 \end{pmatrix}, \tag{12}$$

The normalization factors N and combination coefficients C_i in the expression (10) of $\psi^{\Gamma}_{\mu\nu}$ are listed in Table I.

Table I

The group $\mathbf{I}_h$ is the direct product of $\mathbf{I}$ and the inversion group $\{E, P\}$, where P is the inversion operator. According to the parity, the irreducible representations of $\mathbf{I}_h$ are denoted as Γ_g (even) and Γ_u (odd) with the following irreducible bases:

$$\psi^{\Gamma_g}_{\mu\nu} = 2^{-1/2} (E + P) \psi^{\Gamma}_{\mu\nu}, \qquad \psi^{\Gamma_u}_{\mu\nu} = 2^{-1/2} (E - P) \psi^{\Gamma}_{\mu\nu}. \tag{13}$$

Now we are in the position to construct the symmetry adapted bases (SAB). For a given polyatomic molecule with $\mathbf{I}$ or $\mathbf{I}_h$ symmetry, its vibrational states are described by the vibration quanta occupying in its bonds. Applying the irreducible bases $\psi^{\Gamma}_{\mu\nu}$ to the vibrational states, we obtain the SAB generally. The only problem is to determine the actions of group elements R on the vibrational states according to the geometric meaning of R. In fact, the action of R only permutes, but does not change the vibration quanta. When some quanta are equal to each other, some SAB may be vanishing, or linearly dependent on other states. Let us give three examples to explain the general method of calculating SAB.

Ex. 1. The eigenvalues and eigenfunctions of the Hückel Hamiltonian for Carbon-60.

Deng and Yang (1992) have calculated this problem by computer. Now we calculate the same problem in terms of the irreducible bases $\psi^{\Gamma}_{\mu\nu}$ even by hand. It is easy to see from Fig. 1 in Deng and Yang (1992) that there is one-to-two correspondence between their states $|a,b,c\rangle$ and the group elements R and PR' of $\mathbf{I}_h$ in the following meaning:

$$R\ |1,0,1\rangle = PR'\ |1,0,1\rangle = |a,b,c\rangle, \qquad R \ \text{ and } \ PR' \ \longrightarrow \ |a,b,c\rangle. \tag{14}$$

where $R \in \mathbf{I}$ and $R' \in \mathbf{I}$. Introduce the new notation for the states:

$$|R\rangle = P\ |R'\rangle = |PR'\rangle \equiv |a,b,c\rangle, \qquad P\ |a,b,c\rangle = |\overline{a},b,c\rangle, \tag{15}$$

where the correspondence between $|a=1,b,c\rangle$ and the elements R and PR' of $\mathbf{I}_h$ is listed as follows:

$$|R\rangle = |1,b,c\rangle, \qquad |R'\rangle = |\overline{1},b,c\rangle. \tag{16}$$

$R(R')$	$c=1$	$c=2$	$c=3$	$c=4$	$c=5$	$c=6$
$b=0$	$E(S_{12})$	$S_1(S_8)$	$R^2_5(T^2_4)$	$R_1(T^3_3)$	$T^4_5(R_9)$	$T_2(R^2_7)$
$b=1$	$T_0(S_{15})$	$R^2_1(T^3_4)$	$T^4_1(S_9)$	$S_2(R^2_8)$	$T_3(T^2_5)$	$R_2(R_{10})$
$b=2$	$T^2_0(S_{13})$	$T^4_2(R^2_9)$	$T_4(T^3_5)$	$R^2_2(R_6)$	$R_3(S_{10})$	$S_3(T^2_1)$
$b=3$	$T^3_0(S_{11})$	$T_5(R_7)$	$R_4(R^2_{10})$	$T^4_3(T^2_2)$	$S_4(T^3_1)$	$R^2_3(S_6)$
$b=4$	$T^4_0(S_{14})$	$R_5(T^2_3)$	$S_5(R_8)$	$T_1(S_7)$	$R^2_4(R^2_6)$	$T^4_4(T^3_2)$

Substituting (16) into (8), we obtain:

$$P\ |\Phi^{(1)}_{\mu\mu}\rangle = \eta^{2\mu}\ |\Phi^{(2)}_{\mu\overline{\mu}}\rangle, \qquad P\ |\Phi^{(3)}_{\mu\nu}\rangle = \eta^{2\mu-\nu}\ |\Phi^{(4)}_{\mu\overline{\nu}}\rangle. \tag{17}$$

Thus, some bases in (13) become vanishing or linearly dependent on other bases. The independent bases are listed as follows:

$$\begin{array}{llll}
2^{-1/2}\ |\psi^{A_g}_{00}\rangle = |\psi^{A}_{00}\rangle, & |\psi^{T_{1g}}_{\mu 1}\rangle = |\psi^{T_{1g}}_{\mu\overline{1}}\rangle, & |\psi^{T_{1u}}_{\mu 1}\rangle = -|\psi^{T_{1u}}_{\mu\overline{1}}\rangle, & 2^{-1/2}\ |\psi^{T_{1u}}_{\mu 0}\rangle = |\psi^{T_1}_{\mu 0}\rangle, \\
|\psi^{T_{2g}}_{\mu 2}\rangle = -|\psi^{T_{2g}}_{\mu\overline{2}}\rangle, & |\psi^{T_{2u}}_{\mu 2}\rangle = |\psi^{T_{2u}}_{\mu\overline{2}}\rangle, & 2^{-1/2}\ |\psi^{T_{2u}}_{\mu 0}\rangle = |\psi^{T_2}_{\mu 0}\rangle, & |\psi^{G_g}_{\mu 2}\rangle = |\psi^{G_g}_{\mu\overline{2}}\rangle, \\
|\psi^{G_g}_{\mu 1}\rangle = |\psi^{G_g}_{\mu\overline{1}}\rangle, & |\psi^{G_u}_{\mu 2}\rangle = -|\psi^{G_u}_{\mu\overline{2}}\rangle, & |\psi^{G_u}_{\mu 1}\rangle = -|\psi^{G_u}_{\mu\overline{1}}\rangle, & |\psi^{H_g}_{\mu 2}\rangle = |\psi^{H_g}_{\mu\overline{2}}\rangle, \\
|\psi^{H_g}_{\mu 1}\rangle = -|\psi^{H_g}_{\mu\overline{1}}\rangle, & 2^{-1/2}\ |\psi^{H_g}_{\mu 0}\rangle = |\psi^{H}_{\mu 0}\rangle, & |\psi^{H_u}_{\mu 2}\rangle = -|\psi^{H_u}_{\mu\overline{2}}\rangle, & |\psi^{H_u}_{\mu 1}\rangle = |\psi^{H_u}_{\mu\overline{1}}\rangle.
\end{array} \tag{18}$$

where an additional normalization factor $2^{-1/2}$ has to be introduced when

$$|\psi^{\Gamma}_{\mu 0}\rangle = P|\psi^{\Gamma}_{\mu 0}\rangle \quad \text{ or } \quad |\psi^{\Gamma}_{\mu 0}\rangle = -P|\psi^{\Gamma}_{\mu 0}\rangle.$$

There are 90 bonds that are divided into two types (Deng and Yang 1992). The hp bonds separate a hexagon from a pentagon, and the others are called the hh bonds. Following the notation in Deng and Yang (1992), the Hückel interaction of the 60 hp bonds are equal to $-\alpha$, and that of the 30 hh bonds equal to $(\alpha-2)$. Now, since the states of C_{60} are denoted by the elements R of $\mathbf{I}$, the action of Hamiltonian on the states can be written from (16) and the Figure in Deng and Yang (1992), for example:

$$\begin{aligned}
H\ |E\rangle &= -\alpha\ |T_0\rangle - \alpha\ |T_0^4\rangle + (\alpha-2)\ |S_1\rangle,\\
H\ |T_0\rangle &= -\alpha\ |E\rangle - \alpha\ |T_0^2\rangle + (\alpha-2)\ |R_1^2\rangle,\\
H\ |T_0^4\rangle &= -\alpha\ |E\rangle - \alpha\ |T_0^3\rangle + (\alpha-2)\ |R_5\rangle,\\
H\ |S_1\rangle &= -\alpha\ |R_1\rangle - \alpha\ |R_5^2\rangle + (\alpha-2)\ |E\rangle.
\end{aligned} \tag{19}$$

We are only interested in the properties of H acting on $|E\rangle$ and vice versa. The matrix of the Hamiltonian in the irreducible bases (18) is a hermitian and block one, which can be calculated by the standard method of group theory (Hamermesh 1962). For example, there are two sets of bases $|\psi_{\mu 1}^{T_{1u}}\rangle$ and $|\psi_{\mu 0}^{T_1}\rangle$ for the representation T_{1u}:

$$\begin{aligned}
|\psi_{11}^{T_{1u}}\rangle &= 8^{-1/2}\left\{|\Phi_{11}^{(1)}\rangle - \eta^2|\Phi_{1\overline{1}}^{(2)}\rangle - p^{-1}|\Phi_{11}^{(3)}\rangle + p\eta^2|\Phi_{1\overline{1}}^{(3)}\rangle - p|\Phi_{11}^{(4)}\rangle + p^{-1}\eta|\Phi_{1\overline{1}}^{(4)}\rangle\right\}\\
&= (200)^{-1/2}\ \left\{\sqrt{5}\left(|E\rangle + \eta^{-1}|T_0\rangle + \eta|T_0^4\rangle\right) + (-p^{-1}+p)|S_1\rangle + \cdots\right\},\\
|\psi_{10}^{T_1}\rangle &= 2^{-1/2}\left\{-\eta|\Phi_{10}^{(3)}\rangle + \eta^{-2}|\Phi_{10}^{(4)}\rangle\right\} = (50)^{-1/2}\ \left\{-|S_1\rangle + \cdots\right\},\\
|\psi_{01}^{T_{1u}}\rangle &= 2^{-1}\left\{-\eta^{-1}|\Phi_{01}^{(3)}\rangle - \eta|\Phi_{0\overline{1}}^{(3)}\rangle + \eta^2|\Phi_{01}^{(4)}\rangle + \eta^{-2}|\Phi_{0\overline{1}}^{(4)}\rangle\right\} = (10)^{-1}\ \left\{-2|S_1\rangle + \cdots\right\},\\
|\psi_{00}^{T_1}\rangle &= 2^{-1}\left\{|\Phi_{00}^{(1)}\rangle - |\Phi_{00}^{(2)}\rangle + |\Phi_{00}^{(3)}\rangle - |\Phi_{00}^{(4)}\rangle\right\}\\
&= (10)^{-1}\ \left\{\sqrt{5}\left(|E\rangle + |T_0\rangle + |T_0^4\rangle\right) + |S_1\rangle + \cdots\right\},
\end{aligned} \tag{20}$$

where we only list the terms of $|E\rangle$, $|T_0\rangle$, $|T_0^4\rangle$, and $|S_1\rangle$, which are relevant to the calculation. Comparing the coefficients of the term $|E\rangle$ on both sides of the following equations:

$$\begin{aligned}
H\ |\psi_{11}^{T_{1u}}\rangle &= H_{11}\ |\psi_{11}^{T_{1u}}\rangle + H_{01}\ |\psi_{10}^{T_1}\rangle,\\
H\ |\psi_{10}^{T_1}\rangle &= H_{10}\ |\psi_{11}^{T_{1u}}\rangle + H_{00}\ |\psi_{10}^{T_1}\rangle,\\
H\ |\psi_{01}^{T_{1u}}\rangle &= H_{11}\ |\psi_{01}^{T_{1u}}\rangle + H_{01}\ |\psi_{00}^{T_1}\rangle,\\
H\ |\psi_{00}^{T_1}\rangle &= H_{10}\ |\psi_{01}^{T_{1u}}\rangle + H_{00}\ |\psi_{00}^{T_1}\rangle,
\end{aligned} \tag{21}$$

we obtain the submatrix of H for the representation T_{1u}, which is of two dimensions:

$$\begin{aligned}
H^{T_{1u}} &= \frac{1}{2\sqrt{5}}\begin{pmatrix} -\alpha(7-\sqrt{5})+4 & -4(\alpha-2) \\ -4(\alpha-2) & -2\alpha(2\sqrt{5}-1)-4 \end{pmatrix},\\
E^{T_{1u}} &= -\alpha\left(3+\sqrt{5}\right)/4 \pm \frac{1}{4}\left\{18\alpha^2\left(3-\sqrt{5}\right) - 16\alpha\left(5-\sqrt{5}\right) + 64\right\}^{1/2}.
\end{aligned} \tag{22}$$

The advantage of this method is that the eigenfunctions of the Hamiltonian are able to be obtained simultaneously.

In the same way we can easily calculate the submatrices of the Hückel Hamiltonian for other

representations:

$$H^{A_g} = -\alpha - 2, \quad H^{T_{1g}} = -\alpha\left(\sqrt{5}+1\right)/2 + 2, \quad H^{T_{2g}} = \alpha\left(\sqrt{5}-1\right)/2 + 2,$$
$$H^{T_{2u}} = \frac{1}{2\sqrt{5}}\begin{pmatrix} \alpha(7+\sqrt{5})-4 & 4(\alpha-2) \\ 4(\alpha-2) & -2\alpha(2\sqrt{5}+1)+4 \end{pmatrix}, \quad H^{G_g} = \begin{pmatrix} \alpha(\sqrt{5}+1)/2 & -(\alpha-2) \\ -(\alpha-2) & -\alpha(\sqrt{5}-1)/2 \end{pmatrix},$$
$$H^{G_u} = \frac{1}{2\sqrt{5}}\begin{pmatrix} \alpha(\sqrt{5}+1)+8 & 2(\alpha-2) \\ 2(\alpha-2) & \alpha(\sqrt{5}-1)-8 \end{pmatrix}, \quad H^{H_u} = \frac{1}{2\sqrt{5}}\begin{pmatrix} \alpha(7+\sqrt{5})-4 & 4(\alpha-2) \\ 4(\alpha-2) & -\alpha(7-\sqrt{5})+4 \end{pmatrix},$$
$$H^{H_g} = \frac{1}{10}\begin{pmatrix} \alpha(5\sqrt{5}+11)-12 & 4(\alpha-2) & 4\sqrt{3}(\alpha-2) \\ 4(\alpha-2) & -\alpha(5\sqrt{5}-11)-12 & -4\sqrt{3}(\alpha-2) \\ 4\sqrt{3}(\alpha-2) & -4\sqrt{3}(\alpha-2) & -22\alpha+4 \end{pmatrix}. \tag{23}$$

The dimensions of the submatrices H^{Γ} are one or two except for H^{H_g}, so that the energy levels of the Hückel Hamiltonian are able to be calculated by hand:

$$\begin{aligned} &E^{A_g} = -\alpha - 2, \quad E^{T_{1g}} = -\alpha\left(\sqrt{5}+1\right)/2 + 2, \quad E^{T_{2g}} = \alpha\left(\sqrt{5}-1\right)/2 + 2, \\ &E^{T_{2u}} = -\alpha\left(3-\sqrt{5}\right)/4 \pm \frac{1}{4}\left\{18\alpha^2\left(3+\sqrt{5}\right) - 16\alpha\left(5+\sqrt{5}\right) + 64\right\}^{1/2}, \\ &E^{G_g} = \alpha/2 \pm 2^{-1}\left(9\alpha^2 - 16\alpha + 16\right)^{1/2}, \quad E^{G_u} = \alpha/2 \pm 2^{-1}\left(\alpha^2+16\right)^{1/2}, \\ &E^{H_u} = \alpha/2 \pm 2^{-1}\left(13\alpha^2 - 24\alpha + 16\right)^{1/2}, \end{aligned} \tag{24}$$

and E^{H_g} is the root of the following equation:

$$x^3 + 2x^2 + x\left(-6\alpha^2 + 8\alpha - 4\right) + \left(\alpha^3 - 12\alpha^2 + 16\alpha - 8\right) = 0. \tag{25}$$

The results coincide with that given in Deng and Yang (1992) except for a misprint in (32) of Deng and Yang (1992) ($Q_{3'-}$ and Q_{3-} should be switched, but Fig. 2 in Deng and Yang (1992) is correct.)

Ex. 2. The submatrices of the Hückel Hamiltonian for carbon-240.

It can be seen from Fig. 1 of Chou and Yang (1993) that, in comparison with each atom of Carbon-60, Carbon-240 contains three more carbon atoms distributed symmetrically around that carbon atom of Carbon-60. In addition to (a, b, c), we introduce a new index λ to identify those four carbon atoms. The carbon atom in the center is labeled by $\lambda = 1$, the carbon on the hexagon labeled by 2, and the carbons on the two neighbor pentagons labeled by 3 and 4, respectively. Each carbon atom corresponds to a state, denoted by $|a, b, c, \lambda\rangle$, or by a group element R and λ in terms of the generalized notation in (15):

$$\begin{gathered} |R, \lambda\rangle = |PR', \sigma(\lambda)\rangle = |a, b, c, \lambda\rangle, \quad P\,|a, b, c, \lambda\rangle = |\overline{a}, b, c, \sigma(\lambda)\rangle, \\ \sigma(1) = 1, \quad \sigma(2) = 2, \quad \sigma(3) = 4, \quad \sigma(4) = 3. \end{gathered} \tag{26}$$

From (8) we have:

$$P|\Phi^{(1)}_{\mu\mu}, \lambda\rangle = \eta^{2\mu}\ |\Phi^{(2)}_{\mu\overline{\mu}}, \sigma(\lambda)\rangle, \qquad P|\Phi^{(3)}_{\mu\nu}, \lambda\rangle = \eta^{2\mu-\nu}\ |\Phi^{(4)}_{\mu\overline{\nu}}, \sigma(\lambda)\rangle. \tag{27}$$

Following (10), (13) and (18), we are able to combine $|\Phi^{(i)}_{\mu\nu}, \lambda\rangle$ into the SAB $|\Gamma, \mu, \tau\rangle$. For example,

we have three independent SAB for $\Gamma = A_{1g}$ and one for $\Gamma = A_{1u}$:

$$\begin{aligned}
|A_{1g},0,1\rangle &= |\psi^A_{00},1\rangle = 60^{-1/2}\left\{|E,1\rangle + \cdots\right\},\\
|A_{1g},0,2\rangle &= |\psi^A_{00},2\rangle = 60^{-1/2}\left\{|E,2\rangle + |T_0,2\rangle + |T^4_0,2\rangle + \cdots\right\},\\
|A_{1g},0,3\rangle &= 2^{-1/2}\left\{|\psi^A_{00},3\rangle + |\psi^A_{00},4\rangle\right\}\\
&= 120^{-1/2}\left\{|E,3\rangle + |E,4\rangle + |T^4_0,3\rangle + |T_0,4\rangle + |S_1,3\rangle + |S_1,4\rangle + \cdots\right\},\\
|A_{1u},0,1\rangle &= 2^{-1/2}\left\{|\psi^A_{00},3\rangle - |\psi^A_{00},4\rangle\right\}\\
&= 120^{-1/2}\left\{|E,3\rangle - |E,4\rangle + |T^4_0,3\rangle - |T_0,4\rangle + |S_1,3\rangle - |S_1,4\rangle + \cdots\right\},
\end{aligned} \tag{28}$$

In the bases $|R,\lambda\rangle$, the matrix of the Hückel Hamiltonian H is hermitian. We are only interested in the property of H acting on the states $|E,\lambda\rangle$ and vice versa. For bond arrangement (a) we have:

$$\begin{aligned}
H\ |E,1\rangle &= -\alpha\ |E,3\rangle - \alpha\ |E,4\rangle + (\alpha-2)\ |E,2\rangle\\
H\ |E,2\rangle &= -\alpha\ |T_0,2\rangle - \alpha\ |T^4_0,2\rangle + (\alpha-2)\ |E,1\rangle\\
H\ |E,3\rangle &= -\alpha\ |E,1\rangle - \alpha\ |S_1,4\rangle + (\alpha-2)\ |T_0,4\rangle\\
H\ |E,4\rangle &= -\alpha\ |E,1\rangle - \alpha\ |S_1,3\rangle + (\alpha-2)\ |T^4_0,3\rangle
\end{aligned} \tag{29}$$

and for bond arrangement (b):

$$\begin{aligned}
H\ |E,1\rangle &= -\alpha\ |E,3\rangle - \alpha\ |E,4\rangle + (\alpha-2)\ |E,2\rangle\\
H\ |E,2\rangle &= -\alpha\ |T_0,2\rangle - \alpha\ |T^4_0,2\rangle + (\alpha-2)\ |E,1\rangle\\
H\ |E,3\rangle &= -\alpha\ |E,1\rangle + (\alpha-2)\ |S_1,4\rangle - \alpha\ |T_0,4\rangle\\
H\ |E,4\rangle &= -\alpha\ |E,1\rangle + (\alpha-2)\ |S_1,3\rangle - \alpha\ |T^4_0,3\rangle
\end{aligned} \tag{30}$$

Therefore, in the expansions of (28) we only need list 10 relevant states:

$$\begin{aligned}
&|E,1\rangle, \quad |E,2\rangle, \quad |E,3\rangle, \quad |E,4\rangle, \quad |T_0,2\rangle,\\
&|T_0,4\rangle, \quad |T^4_0,2\rangle, \quad |T^4_0,3\rangle, \quad |S_1,3\rangle, \quad |S_1,4\rangle
\end{aligned} \tag{31}$$

From (28), (29) and (30) we obtain the submatrices of the Hückel Hamiltonian for the representations A_{1g} and A_{1u}:

$$H^{A_{1g}}(a) = H^{A_{1g}}(b) = \begin{pmatrix} 0 & \alpha-2 & -\sqrt{2}\alpha \\ \alpha-2 & -2\alpha & 0 \\ -\sqrt{2}\alpha & 0 & -2 \end{pmatrix}, \qquad H^{A_{1u}}(a) = H^{A_{1u}}(b) = 2. \tag{32}$$

In the cases A_{1g} and A_{1u}, the submatrices of H are same for both bond arrangements (a) and (b). There are more SAB belonging to other irreducible representations. However, the calculations are still simple enough to complete by hand. In the following we list the independent SAB for each irreducible representation and the nonvanishing matrix elements of the Hamiltonian .

$$\begin{aligned}
|T_{1g},\mu,\lambda\rangle &= 2^{-1/2}\left\{|\psi^{T_1}_{\mu 1},\lambda\rangle + |\psi^{T_1}_{\mu\overline{1}},\sigma(\lambda)\rangle\right\}, \quad & |T_{2g},\mu,\lambda\rangle &= 2^{-1/2}\left\{|\psi^{T_2}_{\mu 2},\lambda\rangle - |\psi^{T_2}_{\mu\overline{2}},\sigma(\lambda)\rangle\right\},\\
|T_{1g},\mu,5\rangle &= 2^{-1/2}\left\{|\psi^{T_1}_{\mu 0},3\rangle - |\psi^{T_1}_{\mu 0},4\rangle\right\}, & |T_{2g},\mu,5\rangle &= 2^{-1/2}\left\{|\psi^{T_2}_{\mu 0},3\rangle - |\psi^{T_2}_{\mu 0},4\rangle\right\},
\end{aligned} \tag{33}$$

$$\begin{aligned}
|T_{1u},\mu,\lambda\rangle &= 2^{-1/2}\left\{|\psi^{T_1}_{\mu 1},\lambda\rangle - |\psi^{T_1}_{\mu\overline{1}},\sigma(\lambda)\rangle\right\}, \quad & |T_{2u},\mu,\lambda\rangle &= 2^{-1/2}\left\{|\psi^{T_2}_{\mu 2},\lambda\rangle + |\psi^{T_2}_{\mu\overline{2}},\sigma(\lambda)\rangle\right\},\\
|T_{1u},\mu,5\rangle &= 2^{-1/2}\left\{|\psi^{T_1}_{\mu 0},3\rangle + |\psi^{T_1}_{\mu 0},4\rangle\right\}, & |T_{2u},\mu,5\rangle &= 2^{-1/2}\left\{|\psi^{T_2}_{\mu 0},3\rangle + |\psi^{T_2}_{\mu 0},4\rangle\right\},\\
|T_{1u},\mu,6\rangle &= |\psi^{T_1}_{\mu 0},1\rangle, & |T_{2u},\mu,6\rangle &= |\psi^{T_2}_{\mu 0},1\rangle,\\
|T_{1u},\mu,7\rangle &= |\psi^{T_1}_{\mu 0},2\rangle, & |T_{2u},\mu,7\rangle &= |\psi^{T_2}_{\mu 0},2\rangle,
\end{aligned} \tag{34}$$

where λ runs from 1 to 4, and $\sigma(\lambda)$ was given in (26). Since the submatrices of the Hamiltonian are all hermitian, we only list the nonvanishing matrix elements in the up-triangle part (the row index is not larger than the column index).

$$
\begin{aligned}
&H^{T_{1g}}(a)_{22} = H^{T_{1g}}(b)_{22} = H^{T_{1u}}(a)_{22} = H^{T_{1u}}(b)_{22} = -\alpha p, \\
&H^{T_{1g}}(a)_{33} = H^{T_{1g}}(a)_{44} = -H^{T_{1u}}(a)_{33} = -H^{T_{1u}}(a)_{44} = \alpha p/\sqrt{5}, \\
&H^{T_{1g}}(b)_{33} = H^{T_{1g}}(b)_{44} = -H^{T_{1u}}(b)_{33} = -H^{T_{1u}}(b)_{44} = -(\alpha-2)p/\sqrt{5},
\end{aligned}
$$

$$
\begin{aligned}
&H^{T_{1g}}(a)_{55} = -H^{T_{1u}}(a)_{55} = -(\alpha-2) + \alpha/\sqrt{5}, \\
&H^{T_{1g}}(b)_{55} = -H^{T_{1u}}(b)_{55} = \alpha - (\alpha-2)/\sqrt{5}, \\
&H^{T_{1u}}(a)_{77} = H^{T_{1u}}(b)_{77} = -2\alpha, \\
&H^{T_{1g}}(a)_{12} = H^{T_{1g}}(b)_{12} = H^{T_{1u}}(a)_{12} = H^{T_{1u}}(b)_{12} = H^{T_{1u}}(a)_{67} = H^{T_{1u}}(b)_{67} = \alpha - 2, \\
&H^{T_{1g}}(a)_{13} = H^{T_{1g}}(a)_{14} = H^{T_{1g}}(b)_{13} = H^{T_{1g}}(b)_{14} = H^{T_{1u}}(a)_{13} = H^{T_{1u}}(a)_{14} \\
&\quad = H^{T_{1u}}(b)_{13} = H^{T_{1u}}(b)_{14} = -\alpha, \\
&H^{T_{1g}}(a)_{34} = H^{T_{1u}}(a)_{34} = (\alpha-2)\eta^{-1} + \alpha p^{-1}/\sqrt{5}, \\
&H^{T_{1g}}(b)_{34} = H^{T_{1u}}(b)_{34} = -\alpha\eta^{-1} - (\alpha-2)p^{-1}/\sqrt{5}, \\
&-H^{T_{1g}}(a)_{35} = H^{T_{1g}}(a)_{45} = H^{T_{1u}}(a)_{35} = H^{T_{1u}}(a)_{45} = \alpha\sqrt{2/5}, \\
&-H^{T_{1g}}(b)_{35} = H^{T_{1g}}(b)_{45} = H^{T_{1u}}(b)_{35} = H^{T_{1u}}(b)_{45} = -(\alpha-2)\sqrt{2/5}, \\
&H^{T_{1u}}(a)_{56} = H^{T_{1u}}(b)_{56} = -\alpha\sqrt{2}.
\end{aligned}
\tag{35}
$$

After the replacement of $\sqrt{5}$ by $-\sqrt{5}$ from the submatrices for T_1 representation, we obtain those for T_2.

For the representations G and H we have

$$
\begin{aligned}
&|G_g,\mu,\lambda\rangle = 2^{-1/2}\left\{|\psi^G_{\mu 2},\lambda\rangle + |\psi^G_{\mu\overline{2}},\sigma(\lambda)\rangle\right\}, \qquad |G_u,\mu,\lambda\rangle = 2^{-1/2}\left\{|\psi^G_{\mu 2},\lambda\rangle - |\psi^G_{\mu\overline{2}},\sigma(\lambda)\rangle\right\}, \\
&|G_g,\mu,4+\lambda\rangle = 2^{-1/2}\left\{|\psi^G_{\mu 1},\lambda\rangle + |\psi^G_{\mu\overline{1}},\sigma(\lambda)\rangle\right\}, \ |G_u,\mu,4+\lambda\rangle = 2^{-1/2}\left\{|\psi^G_{\mu 1},\lambda\rangle - |\psi^G_{\mu\overline{1}},\sigma(\lambda)\rangle\right\}.
\end{aligned}
\tag{36}
$$

$$
\begin{aligned}
&H^{G_g}(a)_{22} = H^{G_g}(b)_{22} = H^{G_u}(a)_{22} = H^{G_u}(b)_{22} = \alpha p^{-1},\\
&H^{G_g}(a)_{66} = H^{G_g}(b)_{66} = H^{G_u}(a)_{66} = H^{G_u}(b)_{66} = -\alpha p,\\
&H^{G_g}(a)_{33} = H^{G_g}(a)_{44} = -H^{G_g}(a)_{77} = -H^{G_g}(a)_{88}\\
&\quad = -H^{G_u}(a)_{33} = -H^{G_u}(a)_{44} = H^{G_u}(a)_{77} = H^{G_u}(a)_{88} = -\alpha/\sqrt{5},\\
&H^{G_g}(b)_{33} = H^{G_g}(b)_{44} = -H^{G_g}(b)_{77} = -H^{G_g}(b)_{88}\\
&\quad = -H^{G_u}(b)_{33} = -H^{G_u}(b)_{44} = H^{G_u}(b)_{77} = H^{G_u}(b)_{88} = (\alpha-2)/\sqrt{5},\\
&H^{G_g}(a)_{12} = H^{G_g}(a)_{56} = H^{G_u}(a)_{12} = H^{G_u}(a)_{56}\\
&\quad = H^{G_g}(b)_{12} = H^{G_g}(b)_{56} = H^{G_u}(b)_{12} = H^{G_u}(b)_{56} = \alpha-2,\\
&H^{G_g}(a)_{13} = H^{G_g}(a)_{14} = H^{G_g}(a)_{57} = H^{G_g}(a)_{58} = H^{G_u}(a)_{13} = H^{G_u}(a)_{14}\\
&\quad = H^{G_u}(a)_{57} = H^{G_u}(a)_{58} = H^{G_g}(b)_{13} = H^{G_g}(b)_{14} = H^{G_g}(b)_{57} = H^{G_g}(b)_{58}\\
&\quad = H^{G_u}(b)_{13} = H^{G_u}(b)_{14} = H^{G_u}(b)_{57} = H^{G_u}(b)_{58} = -\alpha,\\
&H^{G_g}(a)_{34} = H^{G_u}(a)_{34} = (\alpha-2)\eta^{-2} + \alpha/\sqrt{5},\\
&H^{G_g}(b)_{34} = H^{G_u}(b)_{34} = -\alpha\eta^{-2} - (\alpha-2)/\sqrt{5},\\
&H^{G_g}(a)_{78} = H^{G_u}(a)_{78} = (\alpha-2)\eta^{-1} - \alpha/\sqrt{5},\\
&H^{G_g}(b)_{78} = H^{G_u}(b)_{78} = -\alpha\eta^{-1} + (\alpha-2)/\sqrt{5},\\
&H^{G_g}(a)_{37} = H^{G_g}(a)_{48} = -H^{G_u}(a)_{37} = -H^{G_u}(a)_{48} = \alpha p^{-1}/\sqrt{5},\\
&H^{G_g}(b)_{37} = H^{G_g}(b)_{48} = -H^{G_u}(b)_{37} = -H^{G_u}(b)_{48} = -(\alpha-2)p^{-1}/\sqrt{5},\\
&H^{G_g}(a)_{38} = H^{G_g}(a)_{47} = H^{G_u}(a)_{38} = H^{G_u}(a)_{47} = \alpha p/\sqrt{5},\\
&H^{G_g}(b)_{38} = H^{G_g}(b)_{47} = H^{G_u}(b)_{38} = H^{G_u}(b)_{47} = -(\alpha-2)p/\sqrt{5}.
\end{aligned}
\tag{37}
$$

$$
\begin{aligned}
&|H_g,\mu,\lambda\rangle = 2^{-1/2}\left\{|\psi^H_{\mu 2},\lambda\rangle + |\psi^H_{\mu\overline{2}},\sigma(\lambda)\rangle\right\}, && |H_u,\mu,\lambda\rangle = 2^{-1/2}\left\{|\psi^H_{\mu 2},\lambda\rangle - |\psi^H_{\mu\overline{2}},\sigma(\lambda)\rangle\right\},\\
&|H_g,\mu,4+\lambda\rangle = 2^{-1/2}\left\{|\psi^H_{\mu 1},\lambda\rangle - |\psi^H_{\mu\overline{1}},\sigma(\lambda)\rangle\right\}, && |H_u,\mu,4+\lambda\rangle = 2^{-1/2}\left\{|\psi^H_{\mu 1},\lambda\rangle + |\psi^H_{\mu\overline{1}},\sigma(\lambda)\rangle\right\},\\
&|H_g,\mu,9\rangle = 2^{-1/2}\left\{|\psi^H_{\mu 0},3\rangle + |\psi^H_{\mu 0},4\rangle\right\}, && |H_u,\mu,9\rangle = 2^{-1/2}\left\{|\psi^H_{\mu 0},3\rangle - |\psi^H_{\mu 0},4\rangle\right\},\\
&|H_g,\mu,10\rangle = |\psi^H_{\mu 0},1\rangle,\\
&|H_g,\mu,11\rangle = |\psi^H_{\mu 0},2\rangle.
\end{aligned}
\tag{38}
$$

$$
\begin{aligned}
&H^{H_g}(a)_{22} = H^{H_g}(b)_{22} = H^{H_u}(a)_{22} = H^{H_u}(b)_{22} = \alpha p^{-1},\\
&H^{H_g}(a)_{66} = H^{H_g}(b)_{66} = H^{H_u}(a)_{66} = H^{H_u}(b)_{66} = -\alpha p,\\
&H^{H_g}(a)_{33} = H^{H_g}(a)_{44} = -H^{H_u}(a)_{33} = -H^{H_u}(a)_{44} = -\alpha p^2/5,\\
&H^{H_g}(b)_{33} = H^{H_g}(b)_{44} = -H^{H_u}(b)_{33} = -H^{H_u}(b)_{44} = (\alpha-2)p^2/5,\\
&H^{H_g}(a)_{77} = H^{H_g}(a)_{88} = -H^{H_u}(a)_{77} = -H^{H_u}(a)_{88} = -\alpha p^{-2}/5,\\
&H^{H_g}(b)_{77} = H^{H_g}(b)_{88} = -H^{H_u}(b)_{77} = -H^{H_u}(b)_{88} = (\alpha-2)p^{-2}/5,\\
&H^{H_g}(a)_{99} = -H^{H_u}(a)_{99} = (\alpha-2) + \alpha/5,\\
&H^{H_g}(b)_{99} = -H^{H_u}(b)_{99} = -\alpha - (\alpha-2)/5,\\
&H^{H_g}(a)_{11,11} = H^{H_g}(b)_{11,11} = -2\alpha,\\
&H^{H_g}(a)_{12} = H^{H_g}(a)_{56} = H^{H_g}(a)_{10,11} = H^{H_u}(a)_{12} = H^{H_u}(a)_{56}\\
&\quad = H^{H_g}(b)_{12} = H^{H_g}(b)_{56} = H^{H_g}(b)_{10,11} = H^{H_u}(b)_{12} = H^{H_u}(b)_{56} = \alpha - 2,\\
&H^{H_g}(a)_{13} = H^{H_g}(a)_{14} = H^{H_g}(a)_{57} = H^{H_g}(a)_{58} = H^{H_u}(a)_{13} = H^{H_u}(a)_{14}\\
&\quad = H^{H_u}(a)_{57} = H^{H_u}(a)_{58} = H^{H_g}(b)_{13} = H^{H_g}(b)_{14} = H^{H_g}(b)_{57} = H^{H_g}(b)_{58}\\
&\quad = H^{H_u}(b)_{13} = H^{H_u}(b)_{14} = H^{H_u}(b)_{57} = H^{H_u}(b)_{58} = -\alpha,\\
&H^{H_g}(a)_{34} = H^{H_u}(a)_{34} = (\alpha-2)\eta^{-2} - \alpha p^{-2}/5,\\
&H^{H_g}(b)_{34} = H^{H_u}(b)_{34} = -\alpha\eta^{-2} + (\alpha-2)p^{-2}/5,\\
&H^{H_g}(a)_{78} = H^{H_u}(a)_{78} = (\alpha-2)\eta^{-1} - \alpha p^2/5,\\
&H^{H_g}(b)_{78} = H^{H_u}(b)_{78} = -\alpha\eta^{-1} + (\alpha-2)p^2/5,\\
&H^{H_g}(a)_{37} = H^{H_g}(a)_{48} = -H^{H_u}(a)_{37} = -H^{H_u}(a)_{48} = 2\alpha p/5,\\
&H^{H_g}(b)_{37} = H^{H_g}(b)_{48} = -H^{H_u}(b)_{37} = -H^{H_u}(b)_{48} = -2(\alpha-2)p/5,\\
&H^{H_g}(a)_{38} = H^{H_g}(a)_{47} = H^{H_u}(a)_{38} = H^{H_u}(a)_{47} = -2\alpha p^{-1}/5,\\
&H^{H_g}(b)_{38} = H^{H_g}(b)_{47} = H^{H_u}(b)_{38} = H^{H_u}(b)_{47} = 2(\alpha-2)p^{-1}/5,\\
&H^{H_g}(a)_{39} = H^{H_g}(a)_{49} = -H^{H_g}(a)_{79} = -H^{H_g}(a)_{89}\\
&\quad = -H^{H_u}(a)_{39} = H^{H_u}(a)_{49} = H^{H_u}(a)_{79} = -H^{H_u}(a)_{89} = -\alpha\sqrt{6}/5,\\
&H^{H_g}(b)_{39} = H^{H_g}(b)_{49} = -H^{H_g}(b)_{79} = -H^{H_g}(b)_{89}\\
&\quad = -H^{H_u}(b)_{39} = H^{H_u}(b)_{49} = H^{H_u}(b)_{79} = -H^{H_u}(b)_{89} = (\alpha-2)\sqrt{6}/5,\\
&H^{H_g}(a)_{9,10} = H^{H_g}(b)_{9,10} = -\alpha\sqrt{2}.
\end{aligned}
\tag{39}
$$

The secular equations can be calculated by a standard program in Mathematica, and coincide with those given in Chou and Yang (1993) except for one dropped zero there. The coefficient of the term $\lambda^6\alpha^5$ in Q_{5+} is 100, not 10.

Ex. 3. The symmetry adapted bases of $B_{12}H_{12}$.

A state in $B_{12}H_{12}$ is described by the vibration quanta in the 12 bonds. Those numbers of the vibration quanta are denoted by n_j and m_j for the bonds OA_j and OB_j, $0 \le j \le 5$, respectively. Applying the irreducible bases $\psi^{\Gamma}_{\mu\nu}$ on the states, we obtain the SAB as follows:

$$
\psi^{\Gamma}_{\mu\nu}\ |n_0n_1n_2n_3n_4n_5m_0m_1m_2m_3m_4m_5\rangle, \tag{40}
$$

where the action of a group element R of $\mathbf{I}$ on the state can be calculated from the definition of R

and from Fig. 1. For example,

$$\begin{aligned}
A_0, A_1, A_2, A_3, A_4, A_5 &\xrightarrow{T_0} A_0, A_2, A_3, A_4, A_5, A_1, \\
A_0, A_1, A_2, A_3, A_4, A_5 &\xrightarrow{S_{11}} B_0, B_4, B_3, B_2, B_1, B_5, \\
A_0, A_1, A_2, A_3, A_4, A_5 &\xrightarrow{S_5} A_5, A_4, B_2, B_3, A_1, A_0, \\
A_0, A_1, A_2, A_3, A_4, A_5 &\xrightarrow{S_{10}} B_3, A_5, B_2, B_0, B_4, A_1.
\end{aligned}$$

Under the applications of T_0, S_{11}, S_5 and S_{10}, the state $|n_0n_1n_2n_3n_4n_5m_0m_1m_2m_3m_4m_5\rangle$ becomes:

$$\begin{aligned}
T_0 :&\quad |n_0n_5n_1n_2n_3n_4m_0m_5m_1m_2m_3m_4\rangle, \\
S_{11} :&\quad |m_0m_4m_3m_2m_1m_5n_0n_4n_3n_2n_1n_5\rangle, \\
S_5 :&\quad |n_5n_4m_2m_3n_1n_0m_5m_4n_2n_3m_1m_0\rangle, \\
S_{10} :&\quad |m_3n_5m_2m_0m_4n_1n_3m_5n_2n_0n_4m_1\rangle.
\end{aligned} \tag{41}$$

When 12 quanta are all different from each other, we obtain 60 SAB that are divided into 16 sets with given irreducible representations. If some quanta are equal to each other, the number of the independent sets may decrease. Since the dimensions of the representations are less than 60 for the seven important cases discussed in Chen and Ping (1997), those representations were called non-regular (Chen and Ping 1997).

IV. CONCLUSION

The symmetry adapted bases are very useful in calculating the eigenvalues and eigenstates of a Hamiltonian with given symmetry. From the irreducible bases in the group space of the symmetry group of the system, the SAB can be calculated generally and simply. This is a standard method in group theory (Hamermesh 1962), and widely used in the problems of vibrations of a polyatomic molecule (Lemus and Frank 1994, Ma *et al.* 1996, Chen *et al.* 1996). The explicit form of the irreducible bases of **I** group space are useful in the future calculations for the molecules with **I** and $\mathbf{I}_h$ symmetry.

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